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(54) Title: METHOD OF IDENTIFYING GLYCAN STRUCTURES USING MASS SPECTROMETER DATA

(57) Abstract: A method for characterising the structure or sub-structure of a glycan or glycan derivative, experimentally derives the mass of an unidentified glycan molecule and compares the mass of the unidentified glycan molecule with identified and characterised glycan structures to select candidate structures for the glycan molecule. Next the mass of fragments of the glycan molecule is experimentally derived and theoretical fragmentation of the selected candidates is conducted. The mass of the fragments of the unidentified glycan molecule is matched with the mass of fragments theoretically derived from the candidate structures. Next scoring occurs to produce ranked confidence scores for each of the candidate structures by comparing the masses of the experimentally derived fragments with the masses of the theoretically derived fragments. Two scoring methods are disclosed namely segmentation and correspondence scoring. If insufficient confidence is obtained in the highest ranked score, further including the step of repeating the process by taking into account more complex cleavage patterns in the theoretical fragmentation step, or by obtaining further spectra.

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